

# Numerical Study of Inelastic Scatterings by Time-Dependent Random Potentials in Two-Dimensional Systems

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Diffusion of electrons in a two-dimensional system with time-dependent random potentials is investigated numerically. In the absence of spin-orbit scattering, the conductivity shows universal weak localization correction. In the presence of it, however, the correction to the conductivity weakly depends on the strength of disorder, and becomes vanishingly small close to the metal-insulator transition point.

## 1. Introduction

Transport properties of the two-dimensional disordered electron systems have attracted much attention in recent years. To understand the transport properties of a random system, the concept of quantum interference plays an important role. Effects of quantum interference are suppressed in the presence of the inelastic scattering, for instance, due to the electron-phonon interaction, due to the Coulomb interaction of conduction electrons, or due to the motion of a single impurity atom. The purpose of this paper is to calculate numerically the conductivity of the two-dimensional systems with time-dependent random potentials with and without spin-orbit scatterings, and to demonstrate dephasing by the time-dependent potential.

The two-dimensional system with spin-orbit interactions belongs to the symplectic universality class, and exhibits the Anderson transition. On the other hand, it belongs to the orthogonal universality class without spin-orbit scatterings. The study of the effect of dynamical potential on the conductivity in the critical regime as well as the weakly localized regime gives how the dephasing modifies the quantum interference effects in the above two universality classes.

## 2. Model and Method

We consider the tight-binding Hamiltonian with time-dependent potential  $\varepsilon_i(t)$  on the two-dimensional square lattice:

$$H(t) = - \sum_{(i,j),\sigma,\sigma'} V_{i,\sigma;j,\sigma'} C_{i,\sigma}^\dagger C_{j,\sigma'} + \sum_{i,\sigma} \varepsilon_i(t) C_{i,\sigma}^\dagger C_{i,\sigma}, \quad (1)$$

with the transfer integral in the Ando model[1]

$$V_{i,i+\hat{x}} = \begin{pmatrix} V_1 & V_2 \\ -V_2 & V_1 \end{pmatrix}, V_{i,i+\hat{y}} = \begin{pmatrix} V_1 & -iV_2 \\ -iV_2 & V_1 \end{pmatrix} \quad (2)$$

where  $C_{i,\sigma}^\dagger$  ( $C_{i,\sigma}$ ) denotes a creation (annihilation) operator of an electron at the site  $i$  with spin  $\sigma$  and  $(i,j)$  are the nearest neighboring sites. Here  $\hat{x}$  ( $\hat{y}$ ) denotes the unit vector in the  $x$  ( $y$ )-direction. All the length-scales are measured in units of the lattice constant  $a_0$ . The strength of the spin-orbit interaction is characterized by the parameter  $S = V_2/V$  with  $V = \sqrt{V_1^2 + V_2^2}$ .

In order to take into account the effect of moving potential, we assume that the site-potentials take the form:

$$\varepsilon_{\vec{r}}(t) = \varepsilon_{\vec{r}}(0) \sqrt{2} \cos [\omega t + \theta(\vec{r})], \quad (3)$$

where  $\omega$  is the frequency. Effects of scattering from impurities are introduced through randomness of site energy  $\varepsilon_{\vec{r}}(0)$  and phase  $\theta(\vec{r})$  at  $t=0$  distributed uniformly in the regions,  $|\varepsilon_{\vec{r}}(0)| < W/2$  and  $|\theta(\vec{r})| < \pi$ . We consider the adiabatic case  $\omega \ll V/\hbar$ , where impurities move slower than electrons. The method of the calculations is essentially the same as those in Refs. [2, 3] where we adopt the method based on the fourth-order decomposition of exponential operators[4].

The quantity we observe is the second moment of the wave packet  $\langle r^2(t) \rangle_c$  defined by

$$\langle r^2(t) \rangle_c \equiv \langle |\vec{r}(t)|^2 \rangle - \langle \vec{r}(t) \rangle^2 \quad (4)$$

with

$$\langle r^2(t) \rangle \equiv \int d\Omega r^{d-1} dr r^2 |\psi(\vec{r}, t)|^2, \quad (5)$$

where  $\psi(\vec{r}, t)$  denotes the wave function at time  $t$ , and  $d$  the dimensionality of the system. If the wave function extends throughout the whole system, the second moment is expected to grow in proportion to time  $t$  as  $\langle r^2 \rangle_c = 2dDt$ . Here, the coefficient  $D$  denotes the diffusion coefficient. In contrast, if the wave function is localized, it is clear that the second moment remains finite in the limit  $t \rightarrow \infty$ [3]. In the metallic region the Einstein relation  $\sigma = e^2 \rho(E_F) D$  relates the conductivity  $\sigma$  to the diffusion constant, where  $\rho(E_F)$  is the density of state at Fermi energy  $E_F$ .

### 3. Numerical Results

We have calculated the second moment of the wave packet  $\langle r^2 \rangle_c$  at various random potential strength. The size of the systems are 500 by 500 for the energies  $E_F/V = -1$ . We have carried out an exact diagonalization for the 20 by 20 subsystem at the center of the system and taken the eigenfunction of the subsystem whose eigenvalue is closest to the given energy  $E_F$  as the initial wave packet. By this procedure we can simulate the diffusion of the wave packet whose energy is approximately equal to  $E_F$ .

Fig. 1 gives an example of the calculated second moment for  $\omega = 10^{-2}V/\hbar$ . The second moment is proportional to the time in a wide range up to  $2 \times 10^3 \hbar/V$ . We can evaluate the diffusion constant of this system with least square fit to these data. In the actual simulation, the quantities  $\langle r^2 \rangle_c$  are averaged over at least four samples of random potential distribution. The density of states  $\rho(E_F)$  in the Einstein relation is evaluated from the direct diagonalization or numerical Green's function method for  $\omega = 0$ . We have obtained that  $\rho(E_F) a_0^2 V = 0.281$  and  $0.251$  for  $W/V = 2\sqrt{2}$  and  $4$ , respectively in the orthogonal system  $S = 0$ , and  $\rho(E_F) a_0^2 V = 0.304, 0.267$  and  $0.222$  for  $W/V = 2\sqrt{2}, 4$  and  $4\sqrt{2}$ , respectively in an example of the symplectic system  $S = 0.5$ . The static conductivity obtained by the present method coincides with that by Landauer formula [2].

In Fig. 2 we show examples of the conductivity in the presence (open circles) and absence (filled circles) of spin-orbit interaction as the function of  $\ln \tilde{\omega}$  where  $\tilde{\omega} = \omega/(V/\hbar)$ . In the absence of spin-orbit interaction the conductivity linearly depends on  $\ln \tilde{\omega}$  as

$$\sigma = A \ln \tilde{\omega} + \sigma(0). \quad (6)$$

The coefficients  $A (\approx 0.22)$  calculated by the least square fit to the averaged conductivity, which are shown by the dotted lines, are almost the same among these different disorder cases, although the conductivity  $\sigma(0)$  for  $\omega = 0$  is significantly different from each other. For  $S = 0.5$  the conductivity decreases linearly, takes a minimum on  $\ln \tilde{\omega} \sim -2$ , and then increases with  $\ln \tilde{\omega}$ . For  $W/V = 2\sqrt{2}$

and 4, the absolute value of the slopes on  $\ln \tilde{\omega} < -2$  is almost half of orthogonal case. The slope on  $\ln \tilde{\omega} < -2$  represented by dashed lines slightly decreases with the increase of the disorder  $W/V$ , and then it becomes almost flat for  $W/V = 4\sqrt{2}$ . Note that,  $W/V = 4\sqrt{2} = 5.66 \dots$  is near the

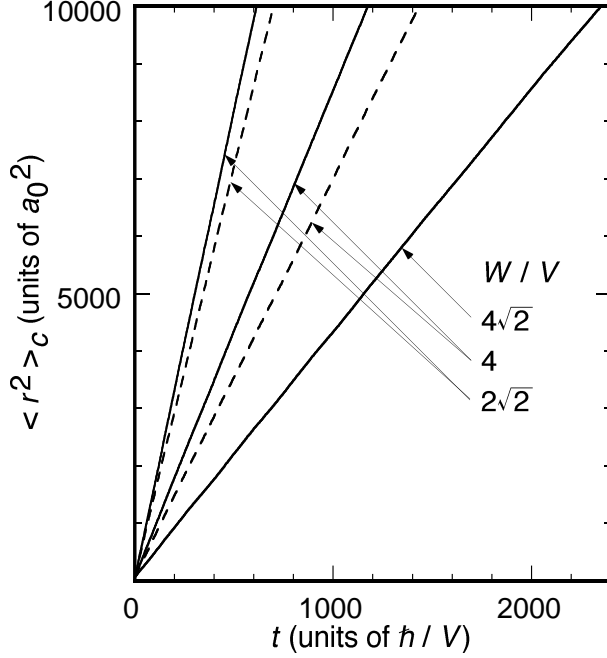


Fig. 1. An example of the second moment as the function of time for  $\omega = 10^{-2}V/\hbar$  and  $E_F/V = -1$ . The dashed line is that in the absence of spin-orbit interactions ( $S = 0$ ) and the solid lines in their presence ( $S = 0.5$ ). The evaluated diffusion constants with least square fit to these data are  $D\hbar/a_0^2V = 3.49$  and  $1.67$  for  $W/V = 2\sqrt{2}$  and  $4$  in  $S = 0$ , and  $D\hbar/a_0^2V = 4.06, 2.11$  and  $1.06$  for  $W/V = 2\sqrt{2}, 4$  and  $4\sqrt{2}$  in  $S = 0.5$ , respectively.

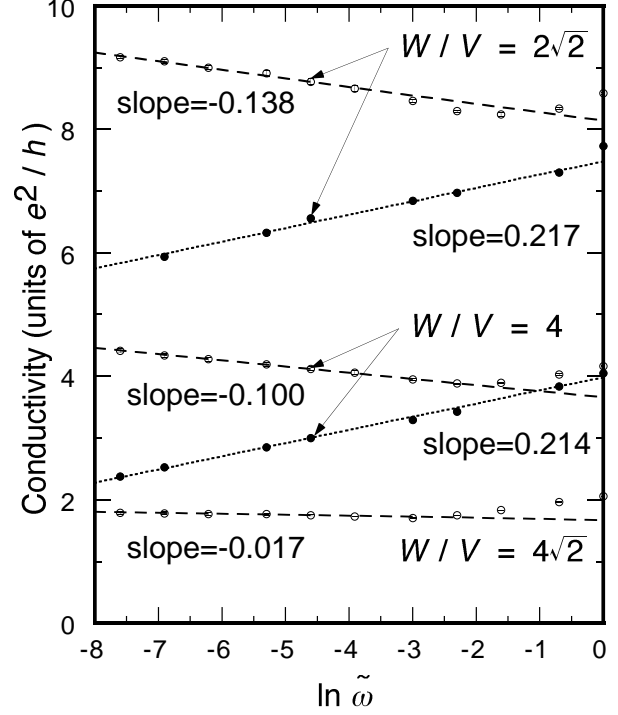


Fig. 2. The calculated conductivity of the two-dimensional system with time dependent impurity potential for  $W/V = 2\sqrt{2}, 4$  and  $4\sqrt{2}$ . The dotted lines indicate in orthogonal system the corrections  $\delta\sigma = 0.217\frac{e^2}{h}\ln\tilde{\omega}$ , and  $\delta\sigma = 0.214\frac{e^2}{h}\ln\tilde{\omega}$ , and the dashed lines in symplectic system the corrections on  $\ln\tilde{\omega} < -2$   $\delta\sigma = -0.138\frac{e^2}{h}\ln\tilde{\omega}$ ,  $\delta\sigma = -0.100\frac{e^2}{h}\ln\tilde{\omega}$ , and  $\delta\sigma = -0.017\frac{e^2}{h}\ln\tilde{\omega}$ , respectively.

critical point of metal-insulator transition  $W_c/V = 5.74$  estimated by the finite-size scaling method for  $E_F = 0$ [1].

#### 4. Discussion and Conclusion

To interpret the above universal correction due to frequency  $\omega$ , we recall the weak localization correction,

$$\delta\sigma = -\frac{e^2}{2\pi^2\hbar} \ln \frac{\tau_\phi}{\tau}, \quad (7)$$

where  $\tau_\phi$  is the dephasing time, and  $\tau$  the elastic scattering time. The  $\omega$  dependence of  $\tau_\phi$  in the kicked rotator problem[5] as well as that in the one-dimensional disordered system [6] in the presence of noise is estimated to be

$$\tau_\phi \sim \omega^{-2/3}. \quad (8)$$

Since the qualitative argument leading to this dependence is independent of the space dimension, the 2D weak localization correction  $\delta\sigma$  [7, 8] is estimated to be

$$\delta\sigma = \frac{2}{3\pi} \frac{e^2}{h} \ln \frac{\omega}{\omega_0}. \quad (9)$$

The pre-factor  $2/3\pi=0.212\dots$  of the  $\ln\omega$  term agrees with the numerical calculation shown in Fig. 2, which is universal and independent of the potential strength  $W$ . Note that this  $\omega$ -dependence is also observed in the case of low energy phonon scattering [9].

The results with the spin-orbit interaction is consistent with the weak localization correction too. For  $\tau_\phi \ll \tau_{SO}$ , where  $\tau_{SO}$  is the dephasing time due to spin-orbit interaction, the conductivity increases with  $\omega$  as in the orthogonal case, while the correction to the conductivity is half with opposite sign for  $\tau_\phi \gg \tau_{SO}$ .

In conclusion, we have analyzed the weak localization effect in the two-dimensional system with time-dependent random potentials using the equation-of-motion method. It has been shown numerically that the weak localization correction to the conductivity due to the fluctuating potentials takes universal value independent of the random potential strength  $W$  in orthogonal system. The symplectic system is also investigated and it is demonstrated that the conductivity becomes almost independent of the frequency near the critical point of metal-insulator transition. Such behavior is observed in the recent experiments with high mobility Si MOS [10], though the mechanism leading to the metal-insulator transition is different. Our results will open a new way to incorporate the dephasing mechanism in numerical simulations.

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## References

- [1] T. Ando, Phys. Rev. **B40** (1989) 5325.
- [2] T. Nakanishi, T. Ohtsuki, and T. Kawarabayashi, J. Phys Soc. Jpn. **66** (1997) 949.
- [3] T. Kawarabayashi and T. Ohtsuki, Phys. Rev. **B51** (1995) 10897; **B53** (1996) 6975.
- [4] M. Suzuki, Phys. Lett. **A146** (1990) 319; **A165** (1992) 387; J. Math. Phys. **32** (1991) 400; J. Phys Soc. Jpn. **61** (1992) 3015; Proc. Jpn Acad. **69**, Ser. B (1993) 161; Commun. Math. Phys. **163** (1994) 491.
- [5] S. Fishman and D. L. Shepelyansky, Europhys. Lett. **16** (1991) 643.
- [6] F. Borgonovi, and D. L. Shepelyansky, Phys. Rev. **E51** (1995) 1026.
- [7] G. Bergmann, Phys. Rep. **107** (1984) 1.
- [8] S. Hikami, A. Larkin and Y. Nagaoka: Prog. Theor. Phys. **63** (1980) 707.
- [9] In the case of low energy phonon scattering, the dephasing time is estimated to be  $\tau_\phi = (3\tau/2mE_F)^{1/3} v^{-2/3}$ , where  $v$  is the phonon velocity. Assuming  $v \propto \omega$  we obtain  $\tau_\phi \sim \omega^{-2/3}$ . See, M. J. Stephen, Phys. Rev. **B36** (1987) 5663. A. A. Golubentsev, Zh. Eksp. Teor. Fiz. **86** (1984) 47. [Sov. Phys. JETP **59** (1984) 26.]
- [10] S. V. Kravchenko, W. E. Mason, G. E. Bowker, J. E. Furneaux, V. M. Pudalov, and M. D'Iorio, Phys. Rev. **B51** (1995) 7038.